Non-Redundant Tensor Decomposition *

Olexiy Kyrgyzov, Deniz Erdogmus
Cognitive Systems Lab
Department of Electrical and Computer Engineering
Northeastern university
Boston, MA 02115
{kyrgyzov,erdogmus}@ece.neu.edu

Abstract

We present the geometrical structure of a basis vector frame for sum-of-rank-1 type decomposition of real-valued tensors. The decomposition we propose reinterprets the orthogonality property of the singular vectors of matrices as a geometric constraint on the rank-1 matrix bases which leads to a geometrically constrained singular vector frame. The proposed approach is essentially a non-redundant one-to-one reparameterization and gives us an upper bound of rank for tensors.

INTRODUCTION. A tensor is a multidimensional array of scalars [3]. An order-p tensor is an element of the space spanned by the outer product of p vectors. The main terms for tensors are the order, dimensions, and the rank. The most widely recognized approaches for sum-of-rank-1 tensor decompositions are: (1) CANDECOMP/PARAFAC (CP) model [2]; (2) the Tucker model [8]. With the CP model, a tensor can be represented as a sum of rank-1 tensors in a unique fashion without any constrains and the dimensionality of this basis set is the rank. Tucker's model factors tensors as a finite sum assuming orthogonal vectors to generate the rank-1 basis tensors similar to SVD, but the result is not necessarily minimal. When we transform data we do not loose information if, at least, our method preserves cardinality of data. SVD preserves cardinality (non-redundant) whereas CP and Tucker models do not follow it (redundant) [4]. This work provides a decomposition model that can decompose any order any dimensionality tensor preserving cardinality.

DECOMPOSITION OF A SYMMETRIC TENSOR. The decomposition of a symmetric tensor $\mathbf{A}$ into a sum of rank-1 tensors utilizes basis tensors that are p-way outer-products of the same vector [7]. Non-redundant decomposition for symmetric tensors was proposed in [5].

Order-2 n-dimensional symmetric tensors. Eigenvector bases for a symmetric n-dimensional order-2 tensor (matrices) are orthogonal, Fig. 1(a). Thus we can decompose it as: $\mathbf{A} = \sum_{l=1}^{n} \lambda_l \mathbf{u}_l^{\circ 2}$, where $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_n]$ is the matrix where columns form an orthogonal frame in n-dimensional space. For numerical decomposition of $\mathbf{A}$ we can use the Jacobi algorithm that tries to find $q = \binom{n}{2}$ rotation angles $\{\theta_k, k = 1, \ldots, q\}$, such that we can construct a rotation matrix $\mathbf{R}(\theta_k)$ in plane $(i,j)\{i = 1, \ldots, n-1, j = i+1, \ldots, n\}$ with angle θ_k (with a one-to-one correspondence between the indices k and (i,j)). This solution consists of q rotation angles and n eigenvalues. The number of free elements of a symmetric n-dimensional matrix $\mathbf{A}$, $m_f(n,2) = n(n+1)/2$, equals the sum $(n+q)$. Consequently, eigendecomposition is simply a reparameterization procedure. Solving for the rotation matrices $\mathbf{R}(\theta_k)$, we can get orthonormal eigenvectors as: $\mathbf{U} = \prod_{k=1}^{q} \mathbf{R}(\theta_k), \mathbf{U}^T\mathbf{U} = \mathbf{U}\mathbf{U}^T = \mathbf{I}$. The eigenvalues are uniquely identified as:

$$\lambda_l = \langle \mathbf{u}_l^{\circ 2}, \mathbf{A} \rangle_F = \sum_{i=1}^{n} \lambda_i \langle \mathbf{u}_l^{\circ 2}, \mathbf{u}_i^{\circ 2} \rangle_F = \sum_{i=1}^{n} \lambda_i (\mathbf{u}_l^T \mathbf{u}_i)^2 \tag{1}$$

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Order-p 2-dimensional symmetric tensors. Let $\mathbf{A}$ be a 2-dimensional order-p symmetric tensor, Fig. 1(b). In an one-to-one reparameterization, the number of linear combination coefficients *r*, plus the number of parameters that characterize *r* corresponding vectors *s*, must be equal to the number of free elements in the tensor; that is $(r + s) = (p + 1)$, since order-p 2-dimensional symmetric tensors have $(p + 1)$ free entries. Incorporating these conditions into the design of the rank-1 sum decomposition, we obtain that symmetric 2-dimensional order-p tensor $\mathbf{A}$ has the following decomposition:

$$\mathbf{A} = \sum_{l=1}^{p} \lambda_l \mathbf{u}_l^{\circ p}, \mathbf{u}_l = \begin{bmatrix} cos(\theta + (l-1)\pi/p) \\ sin(\theta + (l-1)\pi/p) \end{bmatrix} \tag{2}$$

Employing Gram-Schmidt orthogonalization, the linear combination coefficient vector $\boldsymbol{\lambda}$ is uniquely identified by the inner-product matrix between the basis rank-1 symmetric tensor pairs and the inner-product vector between the target tensor and the basis tensors; i.e., at the optimal decomposition, $\boldsymbol{\lambda} = diag(\boldsymbol{\Lambda}) = \mathbf{B}^{-1}\mathbf{c}(\boldsymbol{\theta})$. Here the matrix $\mathbf{B}$ and the vector $\mathbf{c}$ are defined elementwise as in (1):

$$\mathbf{B}_{ij} = \langle \mathbf{u}_i^{\circ p}, \mathbf{u}_j^{\circ p} \rangle_F = \langle \mathbf{u}_i, \mathbf{u}_j \rangle_F^p = (\mathbf{u}_i^T \mathbf{u}_j)^p, \ \mathbf{c}_i(\boldsymbol{\theta}) = \langle \mathbf{u}_i^{\circ p}, \mathbf{A} \rangle_F \tag{3}$$

where $i, j = 1, \ldots, p$ Specifically note that each entry of $\mathbf{B}$ reduces to the following: $\mathbf{B}_{ij} = \cos^p((i-j)\pi/p)$. For symmetric matrices, this matrix is simply identity, $\mathbf{B} = \mathbf{I}$.

Order-p n-dimensional symmetric tensors. The number of free elements of a symmetric n-dimensional order-p tensor, Fig. 1(c), is given by: $m_f(n, p) = \binom{n+p-1}{p}$. The decomposition of any symmetric tensor can consist of some fixed frame of vectors rotated in n-dimensional space and any angle between pairwise vectors can be constant and depends on order p. As in matrices, we need q rotation angles to decompose any symmetric n-dimensional order-p tensor as a finite sum of rank-1 tensors. The number of vectors in this decomposition is: $r = m_r(n, p) = \binom{n+p-1}{p} - \binom{n}{2}$. To obtain the decomposition numerically, we construct a frame of *r* initial vectors placed in columns of a matrix $\mathbf{F}$ and optimize the q rotation angles $\boldsymbol{\theta}$ such that the Frobenius norm of the error tensor is minimized. In the spirit of block coordinate descent and fixed point algorithms, for a given candidate frame orientation, the linear combination coefficients are always obtained using (3) and $\boldsymbol{\lambda} = diag(\boldsymbol{\Lambda}) = \mathbf{B}^{-1}\mathbf{c}(\boldsymbol{\theta})$. At each optimization iteration, basis vectors are expressed as $\mathbf{U} = \left(\prod_{k=1}^{q} \mathbf{R}(\theta_k)\right) \mathbf{F}$.

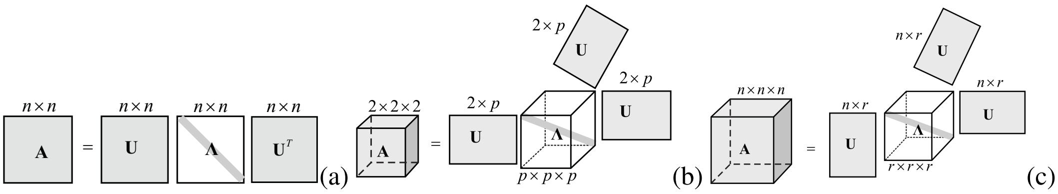

Figure 1: Decomposition of: (a) an order-2 n-dimensional, (b) an order-3 2-dimensional, (c) an order-3 n-dimensional symmetric tensors.

VECTOR FRAMES FOR SYMMETRIC TENSORS. Based on the previous cases of vector frames we can conclude that structure of any vector frame $\mathbf{F}$ must maximize minimal distance between vectors. We can solve this problem by iteratively minimizing the squared error (SE): $e^2 = \langle \mathbf{B} - \mathbf{I}, \mathbf{B} - \mathbf{I} \rangle_F = \sum_{i=1}^{r} \sum_{j=1}^{r} (\mathbf{B}_{ij} - \mathbf{I}_{ij})^2$, where as in (3) $\mathbf{B}_{ij} = (\mathbf{u}_i^T \mathbf{u}_j)^p = (\mathbf{f}_i^T \mathbf{f}_j)^p$. We figured out that for any vector frame planes exist such that frame vectors on those planes separated by π/p radian [4]. This approach gives us r vectors, which yields a full-rank $\mathbf{B}$.

DECOMPOSITION OF A NON-SYMMETRIC TENSOR. The decomposition of a non-symmetric tensor $\mathbf{A}$ into a sum of rank-1 tensors utilizes basis tensors that are p-way outer-products of different vectors.

Order-2 ($\mathbf{n}_1$,$\mathbf{n}_2$)-dimensional non-symmetric tensors. A non-symmetric (n_1,n_2)-dimensional order-2 tensor is a non-symmetric matrix and we have to deal with the common case of SVD.

Singular vector bases for non-symmetric matrices are always selected orthogonal. Thus a full-rank (n_1,n_2)-dimensional non-symmetric matrix can be decomposed as: $\mathbf{A} = \sum_{l=1}^{r} \lambda_l \mathbf{u}_l^{(1)} \circ \mathbf{u}_l^{(2)}$, where r = min(n_1,n_2), $\mathbf{U}^{(1)} = [\mathbf{u}_1^{(1)}, \ldots, \mathbf{u}_r^{(1)}]$ and $\mathbf{U}^{(2)} = [\mathbf{u}_1^{(2)}, \ldots, \mathbf{u}_r^{(2)}]$ are the matrices where columns form orthogonal frames in n_1 and n_2 dimensional spaces, Fig. 2(a). For numerical determination of $\mathbf{A}$ we can use the Jacobi algorithm for each vector frame that tries to find $q = q_1 + q_2$ rotation angles $\{\theta_{k_1}^{(1)}, \theta_{k_2}^{(2)}; k_1 = 1, \ldots, q_1; k_2 = 1, \ldots, q_2\}$, such that we can construct rotation matrices $\mathbf{R}(\theta_{k_1}^{(1)})$ with angle $\theta_{k_1}^{(1)}$ and $\mathbf{R}(\theta_{k_2}^{(2)})$ respectively. Due to cross influence of rotation matrices, $q_1 = \binom{n_1}{2} - \binom{n1-n2}{2}$ and $q_2 = \binom{n_2}{2} - \binom{n2-n1}{2}$, where $\binom{n}{k} = 0$ if $k > n$. This singular decomposition solution consists of $q = q_1 + q_2$ rotation angles and r singular values. The number of free elements of a non-symmetric (n_1, n_2)-dimensional matrix $\mathbf{A}$ equals the product of its dimensionalities so $r = n_1 \cdot n_2 - q$ that satisfies definition of the rank in linear algebra, where $r = min(n_1, n_2)$. Again we can see that singular decomposition is simply a reparameterization procedure. Solving for the rotation matrices $\mathbf{R}(\theta_{k_1}^{(1)})$ and $\mathbf{R}(\theta_{k_2}^{(2)})$, we can get the orthonormal singular vectors given by $\mathbf{U}^{(1)}$ and $\mathbf{U}^{(2)}$ as: $\mathbf{U}^{(i)} = \prod_{k_i=1}^{q_i} \mathbf{R}(\theta_{k_i}^{(i)}),\ (\mathbf{U}^{(i)})^T\mathbf{U}^{(i)} = \mathbf{U}^{(i)}(\mathbf{U}^{(i)})^T = \mathbf{I},\ i = 1, 2$. Due to orthonormality of $\mathbf{U}^{(i)}$, the singular values are uniquely identified as: $\lambda_l = \langle \mathbf{u}_l^{(1)} \circ \mathbf{u}_l^{(2)}, \mathbf{A} \rangle_F = \sum_{i=1}^{r} \lambda_i \langle \mathbf{u}_l^{(1)} \circ \mathbf{u}_l^{(2)}, \mathbf{u}_i^{(1)} \circ \mathbf{u}_i^{(2)} \rangle_F$. Described combination of vectors $\{(1 \circ 1), (2 \circ 2), \ldots, (r \circ r)\}$ is not unique. We can construct $r!$ combinations of vectors on the basis of permutation matrices [1], and any of them can be utilized for (n_1,n_2)-dimensional order-2 non-symmetric tensor decomposition. The permutation matrix is an order-2 r-dimensional binary-matrix that has exactly one entry of 1 in each row and column and 0's elsewhere. In case of symmetry n-dimensional order-2 tensor vectors can be arranged only in ascending order.

Order-p 2-dimensional non-symmetric tensors. Let $\mathbf{A}$ be a 2-dimensional order-p real non-symmetric tensor, Fig. 2(b). As for the case of symmetric 2-dimensional order-p tensor we need r linear combination coefficients plus p rotation angles. Since the number of free elements in order-p 2-dimensional non-symmetric tensors equals to product of dimensionalities, the rank of such a tensor is $r = 2^p - p$. We also know that for each way of tensor we can construct just p vectors. Incorporating these conditions into the design of the rank-1 sum decomposition, we obtain that basis frames for this case of tensor $\mathbf{A}$ are expressed as in (2), where the combinations of vectors $\{(k_l^{(1)}, k_l^{(2)}, \ldots, k_l^{(p)})\}$ for rank-1 tensors must be chosen on the basis of a permutation tensor. Here the permutation tensor is an order-p p-dimensional binary-tensor that has exactly one entry of 1 in each way and 0's elsewhere. The decomposition gives us $\boldsymbol{\lambda} = \mathbf{B}^{-1}\mathbf{c}(\boldsymbol{\Theta})$, where $\boldsymbol{\Theta} = [\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \ldots, \boldsymbol{\theta}^{(p)}]$. Here the matrix $\mathbf{B}$ and the vector $\mathbf{c}$ are defined elementwise as in (3): $B_{ij} = \langle \mathbf{u}_i^{(1)} \circ \mathbf{u}_i^{(2)} \circ \cdots \circ \mathbf{u}_i^{(p)}, \mathbf{u}_j^{(1)} \circ \mathbf{u}_j^{(2)} \circ \cdots \circ \mathbf{u}_j^{(p)} \rangle_F,\ c_i(\boldsymbol{\Theta}) = \langle \mathbf{u}_i^{(1)} \circ \mathbf{u}_i^{(2)} \circ \cdots \circ \mathbf{u}_i^{(p)}, \mathbf{A} \rangle_F$, where $i, j = 1, \ldots, r$.

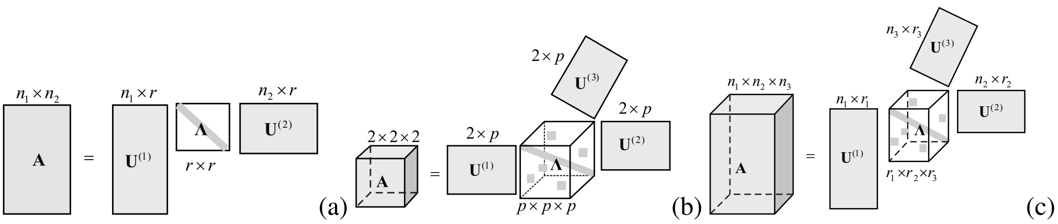

Figure 2: Decomposition of: (a) an order-2 (n_1, n_2)-dimensional, (b) an order-3 $(2, 2, 2)$-dimensional, (c) an order-3 (n_1, n_2, n_3)-dimensional non-symmetric tensors.

Order-p $(\mathbf{n}_1, \mathbf{n}_2, \ldots, \mathbf{n}_p)$-dimensional non-symmetric tensors. The number of free elements of a non-symmetric $(n_1, n_2, \ldots, n_p)$-dimensional order-p tensor, Fig. 2(c), is $m_f(\mathbf{n}, p) = n_1 n_2 \cdots n_p$, where $\mathbf{n} = [n_1, n_2, \ldots, n_p]$. The decomposition of any non-symmetric tensor can consist of some fixed frames of vectors rotated along each way in their dimensionality spaces and any angle between pairwise vectors must be a constant and depends on the order p. As in the case of non-symmetric matrices, we need $q = q_1 + q_2 + \cdots + q_p$ rotation angles. Due to cross influence of rotation matrices: $q_i = \binom{n_i}{2} - \binom{\tilde{n}_i}{2}$; $\tilde{n}_i = n_i - \prod_{j=1, j \neq i}^{p} n_j$ so we can decompose any non-symmetric order-p $(n_1, n_2, \ldots, n_p)$-dimensional tensor as a finite sum of rank-1 tensors. The rank of the tensor in this decomposition is: $r = m_r(\mathbf{n}, p) = m_f(\mathbf{n}, p) - q$. To obtain the decomposition numerically, we construct p frames each of $m_r(n_i, p)$ initial vectors $\mathbf{F}^{(i)}$, $i = 1, \ldots, p$ and optimize the rotation angles $\boldsymbol{\theta}^{(i)}$ such that the Frobenius norm of the error tensor is minimized and $\boldsymbol{\lambda} = \mathbf{B}^{-1}\mathbf{c}(\boldsymbol{\Theta})$. As in the previous case we need to choose r vectors on the basis of an order-p $(r_1, r_2, \ldots, r_p)$-dimensional permutation tensor, where $r_i = m_r(n_i, p),\ i = 1, \ldots, p$. Basis vectors are expressed as $\mathbf{U}^{(i)} = \left(\prod_{k=1}^{q} \mathbf{R}(\theta_k^{(i)})\right) \mathbf{F}^{(i)}$.

NUMERICAL EXPERIMENTS. Iterative optimization technique and application examples are presented in [6, 4]. Here we show numerically that the the upper bound of tensor rank satisfies the proposed decomposition model. Figure 3 shows how decomposition results for non-symmetric order-3 tensors depend on rank and cardinality for best rank-r CP '$\square$', incremental recursive rank-1 CP '$+$', Tucker '$\circ$', and proposed '$*$' models. On the basis of our definitions: in the case of (a), the rank is equal to 5, (c) - 14; in the case of (b), the cardinal number is equal to 8, (d) - 24. Proposed approach gives us the upper bound of CP-rank and the lower bound of cardinality for tensors. The rank-r CP tensor model decomposes data sets with lower tensor rank but utilizes more parameters than cardinality of tensors so it is redundant decomposition.

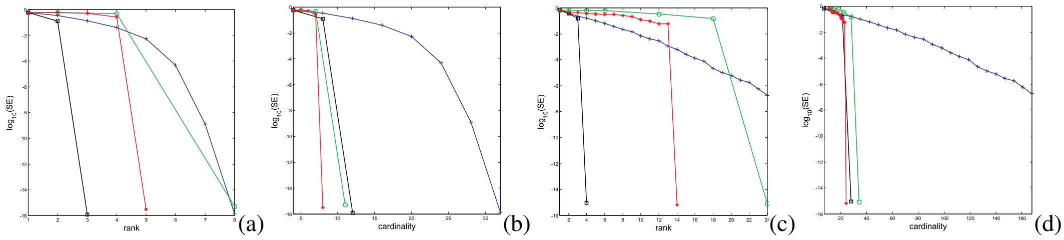

Figure 3: Non-symmetric tensor decomposition SE and corresponding {(a),(c)} tensor rank and {(b),(d)} cardinality for rank-r CP '$\square$', incremental rank-1 CP '$+$', Tucker '$\circ$', and proposed '$*$' models; {(a),(b)} (2,2,2)-dim. tensor; {(c),(d)} (2,3,4)-dim. tensor.

CONCLUSION. We proposed a geometrically constrained basis vector frame that yields a set of rank-1 tensor bases that is able to attain a sum-of-rank-1 tensor decomposition. We described the upper-bound of rank for tensors and used permutation tensors to choose vectors for non-symmetric rank-1 tensor bases from vector bases for symmetric ones. The number of variables that parameterize the proposed decomposition is equal to the number of free elements in the tensor. Future work will decrease complexity and evaluate the properties of the presented decomposition.

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